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Phase transitions of a tethered membrane model on a torus with intrinsic curvature

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Abstract

A tethered surface model is investigated by using the canonical Monte Carlo simulation technique on a torus with an intrinsic curvature. We find that the model undergoes a first-order phase transition between the smooth phase and the crumpled one.

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Keywords: Phase transition; Intrinsic curvature; Elastic membranes

1. Introduction

Recently, it has been growing that the concern with elastic surface models of Helfrich and Polyakov–Kleinert [1–5]. A considerable number of studies have been conducted on the phase transition between the smooth phase and the crumpled one over the past two decades [6–36].

Curvature energies play a crucial role in smoothing the surface. According to curvature energies, surface models can be divided into two classes; one with an extrinsic curvature and the other with an intrinsic curvature. It is also possible that both extrinsic and intrinsic curvatures are included in a model Hamiltonian. Intrinsic curvature is the one that is defined only by using the metric tensor (first fundamental form) of the surface, and extrinsic curvature is defined by using the extrinsic curvature tensor (second fundamental form) of the surface [37]. Both of the mean curvature H and the Gaussian curvature K defined by using the extrinsic curvature tensor, are considered as an extrinsic curvature. However, the Gaussian curvature can also be considered as an intrinsic curvature, because of the relation $2K=R$, where R is the scalar curvature defined only by using the metric tensor.

Intrinsic curvature models were first studied by Baillie et al. in [38–41]. The shape of surfaces can be strongly influenced by intrinsic curvatures. Recently several numerical studies have been made on the phase diagram of the model with intrinsic curvature [23,24]. It was reported that the model undergoes a first-order phase transition between the smooth phase and the crumpled phase on a sphere [23] and on a disk [24]. As a consequence the phase structure of the model has been partly clarified: the transition can be seen independent of whether the surface is compact or non-compact.

However, the model is not yet sufficiently understood. Remaining subject to be confirmed is whether the phase transition and the topology-change are *compatible* in the surface model on compact surfaces. Here *compatible* means that both of two phenomena lead to the same result without depending on which phenomenon firstly occurs. If we define the surface model on compact surfaces, it is reasonable to consider the topology-change of surfaces. In fact, the partition function for the closed string model of Polyakov includes the summation over topology. Moreover, a toroidal vesicle and a genus two vesicle with two holes can be observed in biological membranes [4].

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Therefore, it is interesting, even in the context of the tethered surfaces, to study whether the first-order transition can be observed on a torus, as one of the higher genus surfaces. The phase transition might be seen only on spherical surfaces, if the phase transition and the topology-change are incompatible.

In this Letter, in order to confirm the compatibility we will show that a first-order transition can be seen in the model on a torus with intrinsic curvature and that the phase transition is identical to that observed in the model on a sphere reported in [23].

2. Model

A triangulated real torus is obtained by modifying a triangulated rectangular surface of size $L_1 \times L_2$ as shown in Fig. 1(a). Bending the surface and connecting the sides of length L_1, we have a cylinder of length L_1. Then the remaining two-sides of the cylinder are connected as in the first-step. Thus, we have a real torus as shown in Fig. 1(b), which is topologically identical to the surface in Fig. 1(a) under the periodic boundary condition. The real torus mentioned above will be used in the simulations.

The real torus is, therefore, characterized by the ratio L_1/L_2. Two kinds of tori are used in the simulations: $L_1/L_2 = 2$ and $L_1/L_2 = 4$. Fig. 1(b) is the torus of size $N = 200$ of the first type $L_1/L_2 = 2$, where $L_1 = 20$ and $L_2 = 10$. Every vertex has a coordination number $\sigma = 6$ on the torus.

The Gaussian tethering potential S_1 and the intrinsic curvature S_3 are defined by

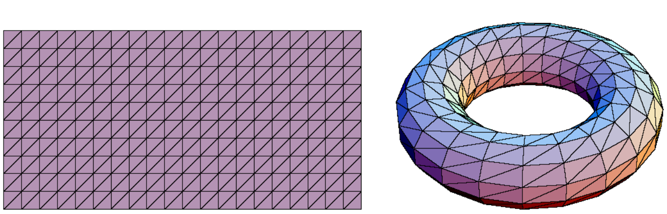
$$S_1 = \sum_{(ij)} (X_i - X_j)^2, \qquad S_3 = -\sum_i \log(\delta_i/2\pi), \tag{1}$$

where $\sum_{(ij)}$ is the sum over bond (ij) connecting the vertices X_i and X_j, and δ_i in S_3 is the sum of angles of the triangles meeting at the vertex i, and $\sum_i$ is the sum over vertices i.

The partition function is defined by

$$Z(\alpha) = \int \prod_{i=1}^{N} dX_i \exp\left[-S(X)\right], \qquad S(X) = S_1 + \alpha S_3, \tag{2}$$

where N is the total number of vertices, which is equal to $L_1 \times L_2$ as described previously. The expression $S(X)$ shows that S explicitly depends on the variable X. The coefficient α is a modulus of the intrinsic curvature. The surfaces are allowed to self-intersect, and the center of each surface is fixed in the partition function $Z(\alpha)$ to remove the translational zero-mode.



(a) (b)

Fig. 1. (a) Rectangular surface of size $L_1 \times L_2 = 20 \times 10$, and (b) the real torus obtained by connecting the opposite sides of the surface in (a).

We note, as described in [23], that the intrinsic curvature term $S_3 = -\sum_i \log(\delta_i/2\pi)$ comes from the integration measure $\prod_i dX_i q_i^{\alpha}$ [42] in the partition function for the model on a sphere, where q_i is the co-ordination number of the vertex i. The term $S_3 = -\sum_i \log(\delta_i/2\pi)$ becomes minimum when $\delta_i = 2\pi$ for all i, and hence it becomes smaller on a smooth torus than on a crumpled one. It is also exact that the term $S_3 = \sum_i (\delta_i - 2\pi)^2$ can be minimized on smooth configurations of the torus. The reason for using the term $S_3 = -\sum_i \log(\delta_i/2\pi)$, as an intrinsic curvature on the torus as in the model on a sphere [23], is that S_3 is closely related to the previously mentioned integration measure.

3. Monte Carlo technique

We use two groups of surfaces classified by the ratio L_1/L_2 in the simulations as mentioned above. The first is characterized by $L_1/L_2 = 2$ and is composed of surfaces of size $N = 1800$, $N = 3200$, $N = 5000$, and $N = 9800$. The second is characterized by $L_1/L_2 = 4$ and is composed of surfaces of size $N = 1762$, $N = 3600$, $N = 6400$, and $N = 10000$.

The variables X are updated by using the canonical Monte Carlo technique so that $X' = X + \delta X$, where the small change δX is made at random in a small sphere in $\mathbf{R}^3$. The radius δr of the small sphere is chosen at the start of the simulations to maintain the rate of acceptance r_X for the X-update as $0.4 \leqslant r_X \leqslant 0.6$.

The total number of MCS (Monte Carlo sweeps) after the thermalization MCS is about 1.5×10^8 in the smooth phase at the transition point of surfaces of $N \geqslant 5000$, and about 1.2×10^8 for the smaller surfaces. Relatively smaller number of MCS (0.8×10^8–1.5×10^8) is iterated in the crumpled phase, because if the surfaces become once crumpled they hardly return smooth. This irreversibility was also seen in the model on a sphere [23] and in the model on a disk [24].

A random number called Mersenne Twister [43] is used in the MC simulations. We use two sequences of random numbers; one for 3-dimensional move of vertices X and the other for the Metropolis accept/reject in the update of X.

4. Results

Figs. 2(a) and (b) show S_1/N against α obtained on the type $L_1/L_2 = 2$ surfaces and on the type $L_1/L_2 = 4$ surfaces, respectively. We find from these figures that the expected relation $S_1/N = 1.5$ is satisfied. Scale invariance of the partition function predicts that $S_1/N = 1.5$. We expect that this relation should not be influenced by whether the phase transition is of first order or not.

The size of surfaces can be reflected in the mean square size X^2 defined by

$$X^2 = \frac{1}{N} \sum_i (X_i - \bar{X})^2, \qquad \bar{X} = \frac{1}{N} \sum_i X_i. \tag{3}$$

In fact, it is expected that the surfaces become smooth in the limit $\alpha \to \infty$ and crumpled in the limit $\alpha \to 0$. In order to see how large the size of surfaces of the type $L_1/L_2 = 2$ is, we plot